

THE SUBMILLIMETER-WAVE SPECTRUM OF ISOTOPIC METHYL CYANIDE¹

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ABSTRACT

The laboratory submillimeter-wave rotational spectrum of the $^{13}\text{CH}_3\text{CN}$, $\text{CH}_3^{13}\text{CN}$, and the $\text{CH}_3\text{C}^{15}\text{N}$ isotopomers of methyl cyanide has been observed in natural abundance in the 294 to 607 GHz region. The maximum J and K values are 34 and 14, respectively. Fifteen additional CH_3CN transitions up to $K=21$ were also measured. The transitions of all four species are fitted to a symmetric top Hamiltonian and the rotation and distortion constants are determined. The ^{14}N quadrupole and spin rotation coupling constants are also calculated and presented. Suggested values for many other parameters which could not be directly determined from the isotope spectra are calculated from the normal species values and isotope relationships. The determined and calculated constants should predict the spectrum of the three isotopomers to well over 1 THz accurately enough for astronomical assignments.

Subject headings: interstellar molecules - laboratory spectra - line identification - molecular processes

1. INTRODUCTION

Methyl cyanide or acetonitrile is a well known interstellar molecule with densities in some sources exceeding $1 \times 10^6 \text{ cm}^{-3}$ (Sutton et al. 1986). The normal species was first detected in the interstellar medium by Solomon, Jefferts, Panzias, & Wilson (1971). Since that time rotational transitions of the two singly substituted ^{13}C isotopes (Cummins et al. 1983 and Sutton et al. 1985), the $365.015965(12) \text{ cm}^{-1}$ (Koivusaari, Horneman, & Anttila 1992) $\nu_8=1$ bending state of CH_3CN (Goldsmith et al. 1983), and the CH_2DCN species (Gerin et al. 1992) have been observed. Methyl cyanide has been detected in nearby galaxies (Mauersberger et al. 1991) and used to make maps of star forming regions (e.g. Habbling & Macdonald 1991 and Olmi, Cesaroni, & Walmsley 1993). Rotational temperatures of over 200 Kelvin (e.g. Sutton et al. 1986) have been reported in some hot cores. At such high temperatures, CH_3CN significantly populates states which have transitions far into the submillimeter region. The rapid development of very sensitive receivers working far into the submillimeter and their use in surveys of hot sources has provided an urgent need to extend the range of quantum numbers where species known to exist in these sources can be accurately predicted.

Methyl cyanide is a textbook example of a prolate symmetric top featuring a large dipole moment, $\mu_0 = 3.92197(13) \text{ Debye}$ (Gadhi et al. 1995) and $\mu_0 = 3.9256(7)$ for $\text{CH}_3\text{C}^{15}\text{N}$ (Mite, Sakai, & Katayama 1984). Since it is a symmetric top (C_{3v} symmetry), it features closely spaced transitions at very different energies in two distinct non-interacting symmetries A and E with $K=3n$ and $K \neq 3n$ ($n=0, 1, 2, 3, \dots$), respectively. The high abundance of CH_3CN and its symmetric top spectral pattern makes it an excellent probe of temperature and excitation in a number of regions (e.g. Cummins et al. 1983, Loren & Mundy 1984, Sutton et al. 1986, and Bishop 1990.). The relative abundance of the A and E symmetries has also been a subject of interest (e.g. Sutton et al. 1986). The transitions of the $\text{CH}_3^{13}\text{CN}$ species closely track the normal species with the $K=0$ transitions in the submillimeter typically appearing near the $K=6$ normal species transition.

The $1\text{T}113\text{-N}$ and the $\text{CH}_3\text{C}^{13}\text{N}$ species have transitions appearing in the same spectral regions but are well separated from the normal species due to their smaller B rotational constants.

Methyl cyanide was one of the first molecules studied with microwave spectroscopy (Ring et al. 1947). A thorough summary of investigations before 1980 was published by Boucher et al. (1980). Between 1980 and now the normal species measurements were extended well into the submillimeter with a variety of techniques (Bocquet et al. 1988, Pavone et al. 1990, Carlotti, Di Lorenzo, & Fusina 1988, and Brown, Dangoisse, & Demaison 1988). With the exception of some Russian work without published transition frequencies, CH_2DCN was the only isotope to be studied in the submillimeter region (Le Guennec et al. 1992) and subsequently observed (Gerin et al. 1992). In this paper, we report submillimeter measurements of the $^{13}\text{CH}_3\text{CN}$, $\text{CH}_3^{13}\text{CN}$ and $013\text{-}1\text{ N}$ isotopomers. In addition to the isotopic species we report a thorough analysis of the normal species including a few new high K transitions. The higher order 013C-N parameters are used in conjunction with isotope relations to derive a suggested set of higher order constants for the isotopic species. Predictions through $J=99$ for methyl cyanide and its isotopomers are too lengthy to publish here, but they are available on-line from the JPL spectral line catalog at spec.jpl.nasa.gov or by anonymous ftp at the same site.

2. EXPERIMENTAL.

The sample of CH_3CN was obtained commercially from Matheson, Coleman, and Bell and required no further purification. Measurements were made with tone burst modulation on 100 GHz phase locked klystrons driving point contact harmonic generators. Second derivative detection using a 4.2 K InSb hot electron bolometer was employed. The data were digitized directly by a computer for further analysis. Measurements were made at room temperature in a double pass polarization rotating one meter cell. The details of this

spectrometer system are described elsewhere (Friedl et al. 1995). All measurements were made in natural isotopic abundance at pressures of 1-10 millitorr. Higher pressures resulted in excessive pressure broadening due to the large dipole moment. Measurement accuracy is estimated to be 30 kHz for the strongest low K transitions up to 150 kHz for the weakest transitions.

Initial predictions for the three isotopic species were based on an analysis of the data in Boucher et al. (1980). These predictions facilitated rapid assignment of the observed spectra in the 290 to 442 GHz region. The 606 GHz transitions were predicted with the aid of the newly measured transitions and were once again readily assignable. Initial normal species predictions were the result of an analysis of the existing data discussed in the following section. As expected, only small deviations within the predicted 1σ uncertainty from the initial line positions were observed at the highest K values.

3. ANALYSIS

The CH_3CN analysis used the data in Boucher et al. (1980), Pavone et al. (1990), Bocquet et al. (1988), Kukolich et al. (1978), and Kukolich (1982) along with the 15 newly measured transitions reported in Table 1. The lower resolution measurements from a variety of sources were not included in the analysis. The transitions reported in Kukolich et al. (1978, 1981) with resolved hydrogen hyperfine were averaged according to relative intensities into ^{14}N quadrupole hyperfine components. The $^{13}\text{CH}_3\text{CN}$ analysis used transitions reported in Boucher et al. (1980) and the 55 new measurements reported in Table 2. The $J=1\leftarrow 0$ transition was measured at the University of British Columbia with a Fourier transform microwave spectrometer described in (Xu, Jäger, & Gerry 1992).

The $\text{CH}_3^{13}\text{CN}$ analysis used the transitions reported in Boucher et al. (1980), Kukolich et al. (1978, 1982) and the 39 new measurements reported in Table 3. The measurements of Kukolich et al. (1978, 1981) appear to be slightly less precise than in the normal species due to the additional complication of the ^{13}C spin. The $J=1\leftarrow 0$ transition

was re-measured at the University of British Columbia and was in excellent agreement with the Kukolich et al. (1978) measurements used in the analysis. The $\text{CH}_3\text{C}^{15}\text{N}$ analysis used transitions reported in Boucher et al. (1980) and the 37 newly measured transitions in Table 4. The $J=1 \leftarrow 0$ transition was measured at the University of British Columbia. In addition to the transitions, Tables 1 through 4 include the fitted observed minus calculated, the lower state energy in wavenumbers, and the log base 10 of the line intensity at 300 K, I_{300} , in units of $\text{nm}^2 \cdot \text{MHz}$. The line intensity at temperature '1' is given by

$$I(T) = (8\pi^3 / 3hc) \nu_{ba}^2 S_{ab} \mu_x^2 / T \left[e^{-E''/kT} - e^{-E'/kT} \right] Q_{rs}^{-1}$$

Where ν_{ab} , S_{ab} , μ_x , E'' , E' , and Q_{rs} are the transition frequency, line strength including the 2:1 A to E statistics, the dipole component along the x axis, lower and upper state energies, and the rotation-spin partition function. For brevity, the line intensities given are a sum of all K parity transitions and the major hyperfine components unless resolved. The partition functions Q_{rs} are given explicitly for each isotopomer. ~here are additional low J transitions for all the isotopomers reported in the literature; however, they were found to be of lower resolution and contained no new information.

The analysis included the effects of ^{14}N quadrupole and the spin rotation coupling where resolved, but none of these effects were observed in the submillimeter region. The CH_3CN lines did appear to broaden somewhat at K near J but no splittings could be resolved. The normal species ground state rotation and distortion constants determined were B, D_J , D_{JK} , H_J , H_{JK} , H_{KJ} , L_{JK} , L_{JK} , and L_{JKK} . The rotation and distortion constants determined for the three isotopic species were B, D_J , D_{JK} , L_{JK} , and H_{KJ} . The rotation and distortion constants along with the ^{14}N quadrupole and spin rotation constants derived from the fit are given on Table 5. Additional constants were fixed to the normal species values and are discussed in the following section.

4. DISCUSSION

The rotational constants A , D_K and H_K cannot be determined from the existing microwave spectra and in general cannot be determined from microwave spectra in C_{3v} molecules without the aid of a suitable resonance; however, these values are needed to calculate relative intensities and rotational energies. As a result, it is necessary to use the A , D_K and H_K values determined from the infrared spectroscopy of the ν_8 , $\nu_7+\nu_8$, and $\nu_7+\nu_8-\nu_8$ bands (Anttila et al. 1993). The A values given in Table 5 for the isotopic species were calculated by scaling the measured normal species A value by the ratio of A_n/A_i (n =normal, i =isotopomer) obtained from the ground state average (r_z) structure which accounted for isotope effects on bond lengths determined by Demaison et al. (1979). The measured D_K constants for the normal species were scaled by the ratio of the A 's squared. The H_K constants were not scaled since the scaling is small compared to the uncertainty in this parameter.

In order to generate accurate predictions to over a THz, the H_J values for $^{13}\text{CH}_3\text{CN}$ and $\text{CH}_3\text{C}^{14}\text{N}$ were calculated by scaling the normal species value by the ratio of the D_J constants to the $3/2$ power. The $\text{CH}_3^{13}\text{CN}H_J$ value was fixed to the ground state since the D_J 's were approximately equal. The values of the I_{JJK} , I_{JK} , and I_{JKK} constants are determined for the normal species, but only I_{JJK} has a significant effect on the fit. These constants were included to give a more realistic prediction of the transition frequency uncertainty in the normal species and the transition frequencies in the isotopomers at higher J and K values. Since the values of these parameters are not particularly well determined, the isotopic species I constants were fixed to the normal species values.

The uncertainty in the $C_{||} - C_{\perp}$ spin rotation parameter in CH_3CN was greatly affected by the uncertainty assigned to the lowest J transitions; however, the value was relatively independent of the uncertainties used. In all the weighting schemes tried, the value varied at most 25% of its quoted uncertainty. The $C_{||} - C_{\perp}$ spin rotation parameter could not be determined in either of the two ^{13}C isotopomers and was fixed to the main

isotope, The ^{14}N quadrupole was well determined for all three isotopomers containing ^{14}N . The C_{\parallel} parameter was determined for the main isotope and the two ^{13}C isotopes. The values of the constants determined should predict the spectrum of $^{13}\text{CH}_3\text{CN}$, $\text{CH}_3^{13}\text{CN}$, and $\text{CH}_3\text{C}^{15}\text{N}$ to well over 1 THz with the accuracy required to assign interstellar spectra.

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TABLE 1
Newly Measured CH₃CN Transitions

Transition				Frequency	Uncertainty	Residual	Intensity ^a	Energy ^b
J''	K''	J'	K'	(MHz)	(kHz)	(kHz)	log(I ₃₀₀)	cm ⁻¹
22	12	21	12	403477.022	35	3	-2.92	854.616
22	13	21	13	403284.991	35	-3	-3.51	947.988
22	14	21	14	403077.969	35	8	-3.84	1111.101
22	15	21	15	402856.002	35	-3	-3.87	1253.927
22	16	21	16	402619.201	50	-6	-4.54	1406.433
22	17	21	17	402367.656	60	-0	-4.95	1568.588
22	18	21	18	402101.450	60	4	-5.09	1740.356
22	19	21	19	401820.705	80	31	-5.89	1921.702
22	20	21	20	401525.450	100	10	-6.45	2112.587
22	21	21	21	401215.800	150	-48	-6.86	2312.973
33	11	32	11	605186.502	90	16	-2.74	922.741
33	12	32	12	604922.882	90	-5	-2.68	1036.266
33	13	32	13	604636.828	120	6	-3.25	1159.552
33	14	32	14	604328.356	150	-45	-3.54	1292.573
33	15	32	15	603997.668	150	-74	-3.55	1435.298

^a See text, The partition function to J=99 including the v₈=1 state and the

¹⁴N quadrupole multiplicity is Q_{rs}=41077.6558.

^b [1'eta] energy of the lower state.

TABLE 2

Newly Measured $^{13}\text{CH}_3\text{CN}$ Transitions

J ^a	Transition			K ^a F ^a	Frequency		Uncertainty	Residual	Intensity ^d	Energy ^b
	K ^a F ^a	J ^a	K ^a F ^a		(MHz)	(kHz)				
1	0 1	0	0 1	1	17865.5446	3	-1	-5.69	0.000	
1	0 2	0	0 1	1	17866.8115	5	-6	-5.46	0.000	
1	0 0	0	0 1	1	17868.7098	1	-0	-6.16	0.000	
17	0	16	0	0	303661.278	30	5	-1.70	81.042	
17	1	16	1	1	303655.577	30	5	-1.71	86.017	
17	2	16	2	2	303638.482	30	10	-1.74	100.939	
17	3	16	3	3	303609.971	30	-8	-1.50	125.804	
18	0	17	0	0	321514.576	30	10	-1.64	91.172	
18	1	17	1	1	321508.537	30	5	-1.65	96.146	
18	2	17	2	2	321490.433	30	1	-1.69	111.067	
18	3	17	3	3	321460.269	30	-5	-1.45	135.932	
18	4	17	4	4	321418.074	30	4	-1.83	170.735	
18	5	17	5	5	321363.819	30	-16	-1.94	215.468	
18	6	17	6	6	321297.592	30	-0	-1.77	270.121	
18	7	17	7	7	321219.355	40	-12	-2.22	334.681	
18	8	17	8	8	321129.183	40	-8	-2.40	409.134	
18	9	17	9	9	321027.096	40	-5	-2.31	493.462	
18	10	17	10	10	320913.145	50	8	-2.84	587.647	
18	11	17	11	11	320787.363	60	16	-3.10	691.667	
18	12	17	12	12	320649.760	60	-22	-3.09	805.498	
18	13	17	13	13	320500.493	80	-8	-3.71	929.114	
18	14	17	14	14	320339.577	80	12	-4.05	1062.487	
22	0	21	0	0	392911.212	35	6	-1.48	137.642	
22	1	21	1	1	392903.848	35	5	-1.49	142.616	
22	2	21	2	2	392881.760	35	1	-1.53	157.534	
22	3	21	3	3	392844.951	35	-10	-1.22	182.395	
22	9	21	9	9	392316.434	50	-2	-2.10	539.862	
22	10	21	10	10	392177.404	50	12	-2.62	634.031	
22	11	21	11	11	392023.897	60	-26	-2.86	738.032	
22	12	21	12	12	391856.099	70	8	-2.82	851.843	
22	13	21	13	13	391673.928	100	-41	-3.42	975.437	
24	0	23	0	0	428598.404	45	15	-1.42	164.450	
24	1	23	1	1	428590.382	45	17	-1.44	169.423	
24	2	23	2	2	428566.300	45	4	-1.47	184.340	
24	3	23	3	3	428526.191	45	-1	-1.22	209.198	
24	4	23	4	4	428470.079	45	10	-1.60	243.991	
24	5	23	5	5	428397.947	40	-3	-1.70	288.711	
24	6	23	6	6	428309.865	40	2	-1.53	343.349	
24	7	23	7	7	428205.845	50	-0	-1.97	407.892	
24	8	23	8	8	428085.941	55	2	-2.14	482.324	
24	9	23	9	9	427950.193	50	0	-2.03	566.629	
24	10	23	10	10	427798.671	70	8	-2.54	660.788	
24	11	23	11	11	427631.420	70	6	-2.78	764.779	
24	12	23	12	12	427448.606	100	90	-2.74	875.578	
24	13	23	13	13	427250.033	120	-14	-3.32	1002.159	
34	0	33	0	0	606895.063	80	-14	-1.33	334.185	
34	1	33	1	1	606883.720	80	-60	-1.34	339.154	

TABLE 2 Continued
Newly Measured $^{13}\text{CH}_3\text{CN}$ Transitions

Transition						Frequency	Uncertainty	Residual	Intensity ^a	Energy ^b
J''	K''	F''	J'	K'	F'	(MHz)	(kHz)	(kHz)	log(I ₃₀₀)	cm ⁻¹
34	2		33	2		606849.895	60	1	-1.37	354.062
34	3		33	3		606793.414	60	-20	-1.13	378.904
34	4		33	4		606714.442	70	20	-1.50	413.675
34	5		33	5		606612.910	70	17	-1.60	458.367
34	6		33	6		606488.915	70	25	-1.42	512.969
34	7		33	7		606342.453	90	-13	-1.86	577.470
34	8		33	8		606173.716	1.50	32	-2.02	651.854
34	9		33	9		605982.507	150	-109	-1.90	736.105

^a See text. The partition function to J=99 including the ^{14}N quadrupole multiplicity is $Q_{\text{rs}}=3 \ 1255.7298$.

^b Total energy of the lower state.

Note: F quantum numbers given only if resolved.

TABLE 3
Newly Measured CH₃¹³CN Transitions

Transition				Frequency	Uncertainty	Residual	Intensity ^a	Energy ^b	
J"	K"	J'	K'	(MHz)	(kHz)	(kHz)	log(I ₃₀₀)	cm ⁻¹	
16	0	1	5	0	294156.780	30	-11	-1.72	73.598
16	1	15	1		294151.143	30	-11	-1.73	78.564
16	2	15	2		294134.230	30	-15	-1.17	93.458
16	3	15	3		294106.059	30	-13	-1.53	118.279
18	0	1	7	0	330907.731	35	-4	-1.61	93.835
18	1	17	1		330901.388	35	-10	-1.62	98.800
18	2	17	2		330882.395	35	5	-1.66	113.694
18	3	17	3		330850.714	30	-6	-1.42	138.512
18	4	17	4		330806.400	40	1	-1.80	173.250
18	5	17	5		330749.431	40	-16	-1.91	217.900
18	6	17	6		330679.886	40	1	-1.73	272.45]
18	8	17	8		330503.047	40	-8	-2.37	411.204
18	9	17	9		330395.866	40	10	-2.2"/	495.376
18	10	17	10		330276.191	50	-1	-2.81	589.385
18	11	17	11		330144.109	60	0	-3.0-1	693.210
18	12	17	12		329999.670	70	11	-3.05	806.828
24	0	2	3	0	441118.129	45	-0	-1.4(1	169.254
24	1	2	3	1	441109.700	45	-5	-1.41	174.218
24	2	2	3	2	441084.413	45	-22	-1.46	189.107
24	3	2	3	3	441042.329	45	-1	-1.20	213.918
24	4	2	3	4	440983.392	45	-15	-1.58	248.646
24	5	2	3	5	440907.691	45	0	-1.68	293.2,82
24	6	2	3	6	440815.209	50	-3	-1.50	34"/.81"/
24	7	2	3	7	440706.000	60	-7	-1.94	412.238
24	8	2	3	8	440580.131	60	0	-2.11	486.533-
24	9	2	3	9	440437.610	60	7	-2.00	570.677
24	10	23	10		440278.534	80	21	-2.51	664.659
24	11	23	11		440102.907	100	-4	-2.7/4	768.454
24	12	23	12		439910.808	120	-6	-2.71	882.039
33	0	3	2	0	606279.403	80	28	-1.31	323."/24
33	1	3	2	1	606267.885	80	25	-1.32	328.684
33	2	3	2	2	606233.319	60	1	-1.35	343.564
33	3	3	2	3	606175.786	60	22	-1.11	368.360
33	4	3	2	4	606095.255	100	33	-1.48	403.068
33	5	3	2	5	605991.710	80	-13	-1.68	447.677
33	6	3	2	6	605865.318	80	7	-1.40	502.180
33	7	32	7		605716.052	120	16	-1.84	566.562
33	8	3	2	8	605543.999	120	41	-2.00	640.810
33	9	3	2	9	605349.078	150	-68	-1.88	724.906

^a See text. The partition function to J=99 including the ¹⁴N quadrupole multiplicity is Q_{rs}=30370.2787.

^b Total energy of the lower state.

TABLE 4
Newly Measured CH₃C¹⁵N Transitions

Transition				Frequency	Uncertainty	Residual	Intensity ^a	Energy ^b
J''	K''	J'	K'	(MHz)	(kHz)	(kHz)	log(I ₃₀₀)	cm ⁻¹
1	0	0	0	17844.0556	7	-8	-5.20	0.000
17	0	16	0	303279.456	30	4	-1.69	80.940
17	1	16	1	3032"/3.730	30	3	-1.70	85.915
17	2	16	2	303256.554	30	2	-1."/4	100.838
17	3	16	3	303227.936	30	2	-1.50	1.25.706
18	0	17	0	321110.459	30	-1	-1.64	91.057
18	1	17	1	321104.397	30	-3	-1.65	96.031
18	2	17	2	321086.224	30	2	--1.69	310.954
18	3	17	3	321.055.917	30	-16	-1.44	135.820
18	4	17	4	321013.553	30	6	-1.83	170.626
18	5	17	5	320959.067	30	-12	-1.93	215.362
18	6	17	6	320892.564	30	11	-1.76	270.019
18	7	17	7	320814.00"/	40	12	-2.22	334.585
18	8	17	8	320723.445	45	9	-2.40	409.044
18	9	17	9	320620.916	40	3	-2.30	493.381
18	10	17	10	320506.465	50	-1	--2.83	587.575
18	11	17	11	320380.144	65	4	-3.09	691.60-/
18	12	17	12	320241.988	80	2	-3.08	805.453
22	0	21	0	392418.271	35	-3	-1.51	124.974
22	1	21	1	392410.875	35	-5	-1.52	129.948
22	2	21	2	392388.704	35	1	-1.56	144.868
22	3	21	3	392351.738	35	-14	-1.31	169.732
24	0	23	0	428061.256	40	-0	-1.42	164.243
24	1	23	1	428053.195	40	-4	-1.43	269.216
24	2	23	2	428029.033	40	1	-1.46	184.134
24	3	23	3	427988.762	40	-1	-1.22	208.994
24	4	23	4	427932.413	40	3	-1.60	243.790
24	5	23	5	427859.978	50	-17	-1.70	288.514
24	6	23	6	427771.552	40	4	-1.52	343.156
24	7	23	7	427667.109	50	6	-1.97	407.704
24	8	23	8	427546.693	50	-11	-2.13	482.142
24	9	23	9	427410.352	100	-46	-2.02	566.455
34	1	33	1	606128.257	80	-8	-1.34	338.736
34	3	33	3	606037.612	60	33	-1.12	378.488
34	4	33	4	605958.259	120	-11	-1.50	413.262
34	5	33	5	605856.363	120	8	-1.59	457.958
34	6	33	6	605"/31.895	120	19	-1.41	512.565

^aSee text. '1'repartition function to J=99 is Q_{TS}=10431.6539.

^bJ'total energy Of the lower state.

TABLE 5
Comparison of Derived Constants

Constant	CH ₃ CN Value ^a (MHz)	¹³ CH ₃ CN Value ^a (MHz)	CH ₃ ¹³ CN Value ^a (MHz)	CH ₃ C ¹⁵ N Value ^a (MHz)
A	158099.063(78) ^b	158107.7 ^c	158093.3~	158107.7 ^c
B	9198.899485(64)	8933.30910(43)	91 94.350598(266)	8922.03905(47)
D _J ×10 ³	3.807622(110)	3.62479(36)	3.810165(268)	3<55554(47)
D _{JK} ×10 ¹⁰	1.774104(45)	1.68179(48)	1.766873(206)	1.689689(286)
D _K	2.8318(45) ^b	2.8332 ^c	2.8297 ^c	2.8332 ^c
H _J ×10 ¹⁰	-2.611(147)	-2.426 ^c	-2.611 ^c	-2.356 ^c
H _{JK} ×10 ⁷	10.2354(290)	8.64(59)	10.240(1 17)	9.688(231)
H _{KJ} ×10 ⁶	6. 104(49)	5.33(50)	6.062(144)	5,762(170)
H _K ×10 ³	0.156(72) ^b	0.156 ^c	0.156 ^c	0.156 ^c
L _{JJK} ×10 ¹²	-7.12(31)	-7.12 ^c	-7.12 ^c	-7.12 ^c
L _{JK} ×10 ¹¹	-5.6(14)	-5.6 ^c	-5.6 ^c	-5.6 ^c
L _{KKK} ×10 ¹⁰	-5.2(10)	-5.2 ^c	-5.2 ^c	-5.2 ^c
L ₅ ×eQq	-6.33745(63)	-6.3329(86)	-6.3286(35)	N/A
C ×10 ³	-3.08(84)	-3.08 ^c	-3.08 ^c	N/A
C - C _⊥ ×10 ³	2.223(125)	2.43(151)	2.62(57)	N/A
μ ₀ Debye	3.92197(13) ^d	3.92197 ^c	3.92197 ^c	3.9256(7) ^c

^a One standard deviation in units of last decimal place given.

^b Fixed value from Anttila et al. (1993).

^c Fixed calculated value see text.

^d Fixed value from Gadhi et al. (1995).

^e Fixed value from Mite, Sakai, & Katayama (1984).

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